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Padmakar - Ivan Index in Nanotechnology

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ABSTRACT

In this survey article a brief account on the development of Padmakar-Ivan (PI) index in that applications of Padmakar-Ivan (PI) index in the fascinating field of nano-technology are discussed.

Keywords: Padmakar-Ivan index, graph-theoretical index, topological index, carbon nanotubes, and nanotechnology.

1. INTRODUCTION

In writing this survey article, I am faced with the necessity of providing the readers with the background information about my involvement in graph theory and my graph-theoretical interests. During 1986-1988, I came across several problems connected with chemical topology and graph theory. In 1988 as a recipient of Fulbright award I was at Brigham Young University, Provo, USA where I collected several papers, articles, reviews and some books on graph –theoretical problems related to chemistry. I started learning mathematical aspects of graph theory from my colleagues and friends, namely Professors N. V. Deshpande and P. P. Kale, Department of Mathematics, D. A. University, Indore, India.

In India, my attempts to find graph-theoreticians willing to collaborate with me for doing research in chemical graph theory proved unsuccessful. Then in 1993, I wrote a letter to Professor Ivan Gutman of Yugoslavia and a fruitful cooperation resulted only when Gutman found me illegible for such collaboration. For that he put me several questions: Where did you learn about chemical graph theory? What kind of mathematical background do you have? Did you publish anything in the field of theoretical / mathematical chemistry? Which literature on the above subjects do you possess? Along with these questions Gutman attached his very brief curriculum vitae and to my surprise at his very young age he is

recipient of A. V. Humboldt Fellowships three times for 1977, 1980, 1985; Fulbright fellow two times for 1989, 1990; NTNF Fellow 1988; JSPS Fellow 1989. As a side remark, graph-theoretical chemists have been mostly trained as physical chemists or quantum chemists, with a strong mathematical background. And LOO! Gutman is M.Sc. in chemistry and PhD in chemistry as well as in mathematics. After going through the bio -data of Gutman, I have lost the hope of having collaborative research with him. The obvious reason being at that time I knew very little about graph theory.

Instead of answering aforementioned questions from Gutman, I just send him my full curriculum vitae and my list of publications. In reply, Gutman found me capable of making collaborative research with him and advised me that the study of spectral moments may perhaps be a good starting point. And then with his personal remark "Based on your beautiful results" I (Gutman) completed a paper "***Spectral Moments of Linear Polyacenes"*** This is how the first paper with Gutman and my first publication in chemical graph theory was published in 1994. The Editor–in–Chief of the journal gave very impressive remark as below: …"***The Journal is fortunate to be able to carry strong papers such as yours dealing with spectral moments of polyacene and I would like to thank you for submitting your paper to us. I hope you will continue to consider this to be the journal of choice when you publish your research results in the future***".

Prof. GWA Milne, Editor-in-Chief,
Journal of Chemical Information and Computer Science,
Published by the American Chemical Society, USA.

Another paper on spectral moments also appeared in 1994 which was: **Dependence *of Spectral Moments of Benzenoid Hydrocarbon on Molecular Structure: The Case of Linear Polyacenes*** [2]

During June 1994, Gutman was intended to examine a few Wiener – number related quantities, which can be considered as generalization of Wiener-number concept. One of these quantities is W* [3]. Gutman was attacking the problem of W* of benzenoid chains (un-branched catacondensed Benzenoids). He asked me to join in his unfinished research. This offer from Gutman provided me to learn much more of graph-theoretical / topological indices and other related graph-theoretical concepts [4–9]. The obvious reason for learning more of topological indices being the quantity W* put forward by Gutman happened to be the extension of Wiener –number to cyclic graphs [3].

Unfortunately, the referred offer from Gutman came to me at a very bad time. I had very acquitted difficulties; both at home front as well as in my services. My wife was having serious kidney problem and my Vice Chancellor was unhappy and was angry with me because as a member of Executive Council of my University I did not allow him to

make any illegal and sub-standard appointments. Such difficulties continued for a very long period and ultimately ended in 2006. Almost for this span of life I spend sleepless nights. However, I kept myself busy in reading the literature on graph theory, which I had collected from Provo, USA.

My wife was operated for left-Kidney removal. While attending her in the hospital I discovered a solution to the aforementioned problem related W* and proved that

$$W^*(Ch) = W^*(C'h) \pmod 8 \qquad (1)$$

Gutman was very happy for this solution. This resulted into yet another joint paper: ***The Szeged Index and an Analogy with the Wiener Index*** [10]. This was my first paper on topological indices. Following this several other papers were published with Gutman [11-17].

It is worth mentioning that Gutman in his earlier paper in 1994 [3] had not given any name to W*, it was in the latter paper [10] the name Szeged index was given and abbreviated as Sz. There is a beautiful story behind the discovery of Sz index by Gutman. In 1994; Gutman was at Szeged, a town in Hungary where he conceived the idea of Szeged index. Hence is the name 'Szeged index'.

At this stage it is interesting to mention that topological indices are number associated with chemical structures i.e. with constitutional graphs [4–9]. There is not a one-to-one association with chemical structures and topological indices, because several graphs may have the same topological index, and may be degenerate [4]. Applications of topological indices, a field, which had been initiated by H. Wiener in USA, M. Gordon in England and the Zagreb group consisting of M. Randic, N. Trinajstic, I. Gutman and others, have instituted a very strong field of research in chemical graph theory. Among Romanian workers I will like to site A. T. Balaban, O. Ivanciuc, T. S Balaban, Z. Simon and M. V. Diudea. In addition, I have to site the name of S. J Cyvin. Needless to state that topological indices are useful tools for quantitative structure-activity-property – toxicity relationships (QSAR, QSPR.QSTR).

The first, oldest and even today widely used molecular descriptor is the Wiener number [18], which was then renamed as Wiener index by Hosoya [19]. The Wiener index is principally advocated for acyclic compounds (trees) and it remained unattended for 25 years. It was in 1972 that Hosoya [19] described its calculation using the distance matrix. Since then Wiener index is widely used in QSPR/QSAR/QSTR studies. This index is defined as below:

The *Wiener index* W = W(G) was first defined for a tree G = T by the following expression:

$$W = W(T) = 1/2 * \Sigma d(i, j), \qquad (2)$$

where the summation going over all pairs (i, j) of vertices $i, j \in V(G)$, or by

$$W = W(T) = \Sigma n(i(e))*n(j(e)), \quad (3)$$

where the summation going over all edges $e = (i, j) \in E(G)$.

The *Szeged index* Sz (G) of graph G is defined (see also equations (1), (2)) by

$$Sz(G) = \Sigma n(i(e))*n(j(e)) \quad (4)$$

The right-hand side of Eq.(4) , although formally identical to the right-hand side of eq.(3), differrs in the interpretation of n(i(e)) and n(j(e)). In the former case, eq.(3), they are the number of vertices of G lying on two sides of the edge e. While in case of eq.(4), if we define an edge e = uv, then n(i(e)) is the number of vertices closer to u than v, and n(j(e)) is the number of vertices closer to v than u; vertices equidistant to u and v are not counted. For more details please see references [20-28].

Since Sz and W indices of acyclic graphs coincide, Khadikar to remove this lacuna, proposed another index in 2000, which he named Padmakar-Ivan index and abbreviated as PI [29]. It is worth mentioning that Padmakar is the first name of Khadikar, while Ivan is the first name of Gutman. Khadikar [29] conceived this index while attempting simultaneous estimation of Wiener and Szeged indices of benzenoids using elementary cut method. The Padmakar-Ivan index is defined it as below:

The PI index of a molecular graph is defined by the following expression:

$$PI = PI(G) = \Sigma_{e \in E(G)}[n_{eu}(e \mid G) + n_{ev}(e \mid G)] \quad (5)$$

Here, we define edge of G connecting the vertices u and v, as $e = uv \in E(G)$. The quantities n_{eu} and n_{ev} are the number of edges closer to u and v respectively. In calculating PI index edges equidistance from both end of the edge *uv* are not counted. The PI index of acyclic and cyclic graphs differs. However, the main interest of proposing a topological index for cyclic graph alone remained unresolved.

The PI index was mostly compared with the Wiener and Szeged indices. It turned out that the PI index has similar discriminating power as the other two indices and in many cases PI index gives better results [30]. The Szeged index incorporates the distribution of vertices of a molecular graph; while the PI index does this job for the edges. Hence, it seems that the combination both could give better results. Indeed this was found very true in many cases. For more detail readers are advised to go through the references [30-36].

It is useful to mention that PI index is a more Szeged -like topological index. On the other hand, Szeged and Wiener indices of trees are the same. So, there are some differences among and also similarities of PI, Szeged and Wiener indices, which are quoted here. The PI index is the unique topological index related to parallelism of edges, but the Wiener index is the most important topological index related to distances between vertices. The PI index is very simple to calculate and has disseminating power similar to that of the Wiener and Szeged indices. Khadikar and coauthors investigated numerous chemical and biological applications in that PI index and they found PI index superior to both Wiener and Szeged indices [30, 32].

Once again, in the year 2002 Khadikar has proposed yet another W–Sz–PI like index, which he named Sadhana index and abbreviated as the Sd index [21, 23, 37-43]. At that time no mathematical definition was given to this index. It is in the paper [42] for the first time Khadikar provided such a mathematical definition to the Sd index. It is interesting to mention that Sz, PI and Sd indices are W–like indices having similar decrementing power. The ways in which these indices are proposed clearly indicate that there is one-to-one correlation among these four indices. Also, there is close correspondence in defining these indices as well. The Wiener index counts the number of vertices on both sides of an edge; the Szeged index makes account of number of vertices closer to both the ends of an edge; the PI index on the other hand sum up the number of edges on both the ends of an edge, and finally, Sadhana index sum up the number of edges on both the sides on an elementary cuts.

The *Padmakar-Ivan index* PI(G) for a bipartite *SCO* graph G is defined by (s = 1, 2, c).

$$PI(G) = \Sigma m_s(G) \times (m(G) - m_s(G)). \quad (6)$$

From a simple calculation follow

$$PI(G) = m(G)^2 - \Sigma m_s(G)^2. \quad (7)$$

The *Sadhana index Sd* (G) of a bipartite *SCO* graph G is defined (for summation index s = 1, 2, c) by

$$Sd(G) = \Sigma (m(G) - m_s(G)). \quad (8)$$

For *sco* graph G is $\Sigma m_s(G) = m(G)$ and with definition (6) follow immediately

$$\begin{aligned} Sd(G) &= m(G) * c(G) - m(G) \\ &= m(G) * (c(G) - 1) . \end{aligned} \quad (9)$$

Special Graphs

For a tree G = T is every $m_s(G) = 1$, and $c(T) = m(T)$:

$$\begin{aligned} Sd(T) &= m(T) \times (c(T) - 1) \\ &= m(T) \times (m(T) - m_s(T)) \\ &= m(T)^2 - m(T) \times m_s(G) \\ &= m(T)^2 - c(T) \times m_s(G) \\ &= m(T)^2 - \Sigma ms(T)^2 \\ &= PI(T) \end{aligned} \quad (10)$$

For a circuit G = C of even length is every $m_s(G) = 2$, and $c(C) = \frac{1}{2}m(C)$, and we find

$$\begin{aligned} Sd\ C &= m(C)*(c(C) - 1) \\ &= m(C)* (1/2*m(C) - 1) \\ &= \tfrac{1}{2}*m(C)*(m(C) - 2) \end{aligned}$$

$$= ½*\{m(C)\ ^2 - 2*m(C)\}$$
$$= ½*\{m(C)\ ^2 - (½*m(C))*(2^2)\}\}$$
$$= ½*\{m(C)\ ^2 - \Sigma ms\ (T)^2\}$$
$$= ½*PI(C). \qquad (11)$$

In the existing literature there are numerous reports on applications of the Wiener index; more than 100 applications of the Szeged index; and 50 cases of the PI index in QSAR / QSPR / QSTR and around 100 cases of the applications of PI index in solving the problem related to nanotechnology in particular carbon-nanotubes. Compared to these three indices, in the case of recently introduced Sadhana index lot more investigations are yet to be made.

Carbon nanotubes (CNTs) are peri-condensed Benzenoids, which are ordered in graphite –like, hexagonal pattern. They may be derived from graphite by rolling up the rectangular sheets along certain vectors. All benzenoids, including graphite and CNTs are aromatic structures.

Carbon nanotubes form an interesting class of carbon nano-materials. These can be imagined as rolled sheets of graphite about different axes. There are three types of nanotubes: armchair, chiral and zigzag structures. Furthermore, nanotubes can be categorized as single-walled and multi-walled nanotubes. It is very difficult to produce the former type of nanotubes. In 1991 Lijima [44] discovered carbon nanotubes as multi-walled structures. Carbon nanotubes show remarkable mechanical properties. Experimental studies have shown that they belong to the stiffest and elastic known materials.

One of the main distinctive characteristics of carbon nanotubes is the use of mathematical tools for modeling of their physicochemical properties as well as medical and toxicological effects of carbon nanotubes.

Graph theory is a basic tool to solve these problems, both by the high degree of abstraction evidenced by the generality of such concepts as points, lines and neighborhood as well as by the combinatorial derivation of many graph theoretical concepts. This method offers a wide variety of concepts and procedures of significant importance to carbon nano-technology.

The graph-theoretical characterization of carbon nanotubes in terms of molecular structure is most often made by its translation into molecular graph (MG). In doing so, all the constituting atoms of carbon nanotubes are considered as vertices, while all the bonds involved in them are treated as edges. Thus, carbon nano-technology, a graph G is defined as a finite non-empty V (G) of N-vertices (atoms) together with a set E(G) of edges (bonds), the latter being unordered pairs of distinct vertices (atoms). Then, by definition, every molecular graph of carbon nanotube is finite and has no loops and multiple edges. The graph – theoretical characterization of molecular structure of carbon nanotube Vis–a-vis molecular graph of carbon nanotube is most often made by its translation into molecular

descriptors, such as graph-theoretical descriptors or more precisely topological indices. A topological index is a real number, associated in an arbitrary way, characterizing the graph. It is based on a certain topological feature of the corresponding MG and represents a graph invariant; that is to say, it does not depend on the vertex numbering.

Topological indices of nanotubes, therefore, are numerical descriptors that are derived from graphs of chemical compounds. Such indices based on the distances in a graph are widely used for establishing relationships between the structure of nanotubes and their physicochemical properties and physiological properties of nanotubes.

Diudea was the first chemist who considered the problem of computing topological indices of nanostructures [45-47]. Recently computing topological indices of nanostructures has been the object of many papers. In a series of papers, Diudea and coauthors [45-47] studied the topological indices of some chemical graphs related to nanostructures. In [40, 48-81] Ashrafi and co-authors computed some topological indices of nanotubes. It is worth mentioning that Ashrafi and his group have done voluminous work on the estimation of topological properties of carbon nanotubes. He is the first Iranian scientist working in this field. In Tables 1 and 2, we summarize the references in that PI index is computed for cyclic graphs and related nanotubes by several workers. Below, we mention the types of topological indices, which are used in nanotechnology. In addition to Ashrafi [40, 48-81] several other scientists worked on the applications of PI index in nanotechnology [41, 47, 55, 82-92].

2. GRAPH-THEORETICAL INDICES OF NANOTUBES

Literature survey has indicated that graph-theoretical descriptors, which are used in the study of nanotubes, are Wiener-, Szeged -, PI-, Balaban and Schultz's indices. Only a couple of examples are found for the use of Balaban, Detour, and Schultz indices in nanotechnology. Very large amount of work is done on the applications of PI index in nanotubes. More than 100 papers appeared in the short span of five years. All these papers are concerned with the application of PI index to nanotubes.

Once again, I will like to mention that Ashrafi and his group have done voluminous work on the estimation of topological indices, in particular PI index of carbon nanotubes. Also that, Asharfi is the first Iranian scientist working in the field of nanotechnology. In addition, scientists from other part of the world are also using PI index in nanotechnology. (Table1).

The computation of PI indices of the following nanotubes is reported in the literature:

1. Armchair Polyhex Nanotubes ;
2. Zig-Zag Polyhex Nanotubes;

3. Polyhex Nanotubes;
4. Third and Fourth Dendrimer Nanostars;
5. V-Phenylenic Nanotubes;
6. H-Phenylenic nanotubes;
7. Polyhex Nanotori;
8. V-Phenylenic Nanotori;
9. H-Phenylenic Nanotori;
10. One-pentagonal Carbon Nanotubes;
11. TC4C8® nanotori;
12. TUC4C8 (S) Carbon Nanotubes;
13. HAC5C6C7 Nanotori;
14. HAC5C6C7 Nanotubes;
15. VC5C7 [p.q] Nanotubes;
16. HC5C7 [p.q] Nanotubes, etc.

For further details refer Table 1. Table 2 gives account on the use of Padmakar –Ivan Index (PI) to cyclic graphs related to carbon- nanotubes. Publications related to the use of Padmakar –Ivan index (PI) in developing QSAR/QSPR/QSTR are summarized in Table 3. Table 4 shows institutes wherein research related the applications of PI index to nanotechnology and cyclic graphs related to carbon- nanotubes are in progress.

3. IMPORTANT NANO–STRUCTURES

The important nano-structures for which PI indices were computed are given below:

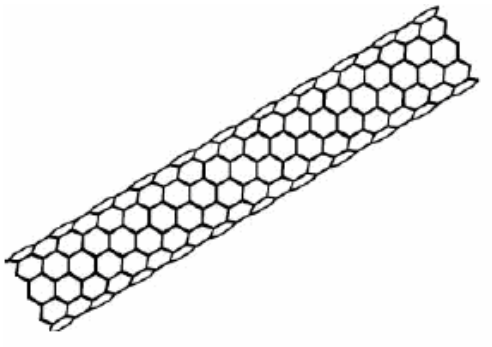


Figure 1. Zig-Zag TUHC6 [20, q].

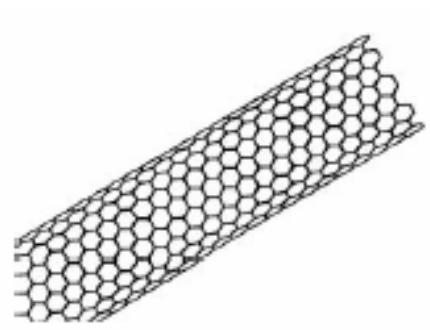


Figure 2. An Armchair TUVC6 [20, n].

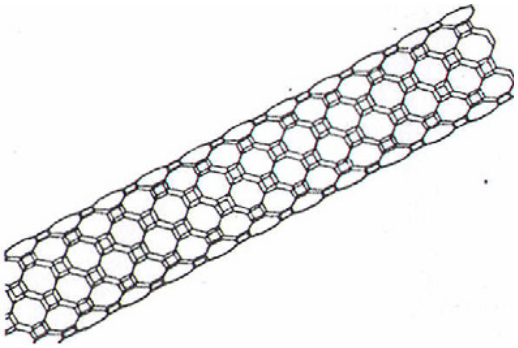


Figure 3. A $TUC_4C_8(S)$ Nanotubes.

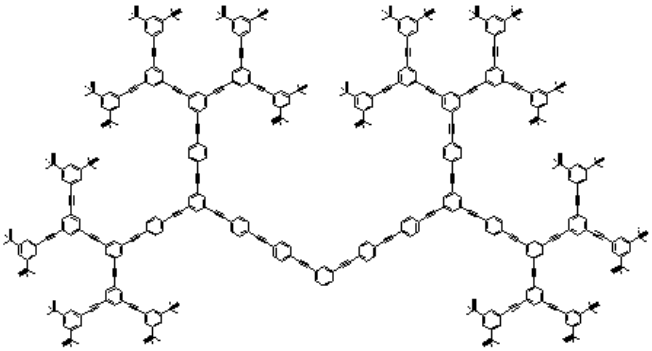


Figure 4. A Nanostar of Type I, with n = 3 and k =1.

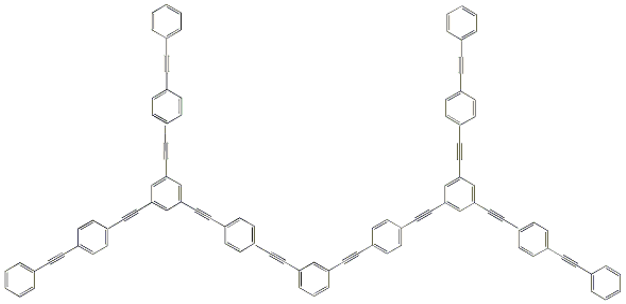


Figure 5. A Nanostar of Type II, with n = 3 and k = 1.

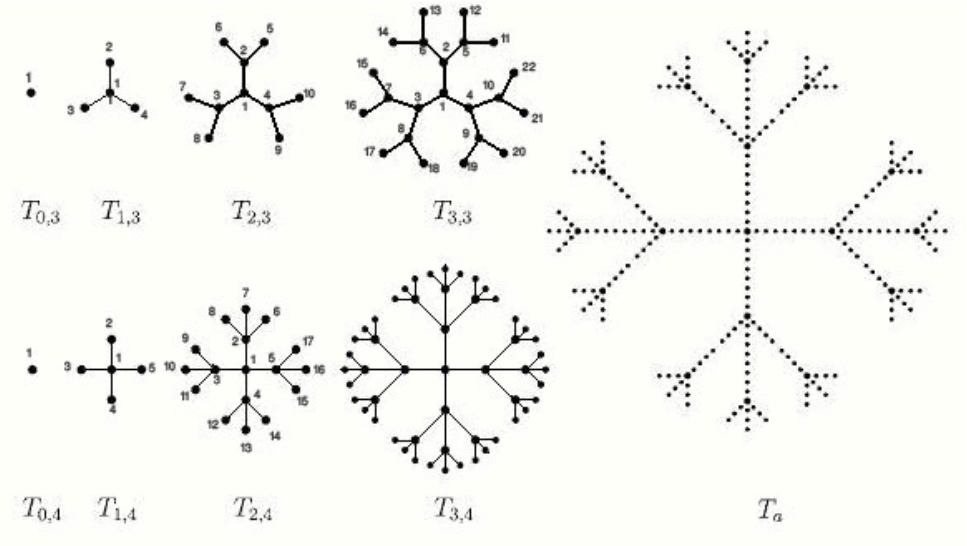


Figure 6. Molecular graphs of dendrimers $T_{K,d}$.

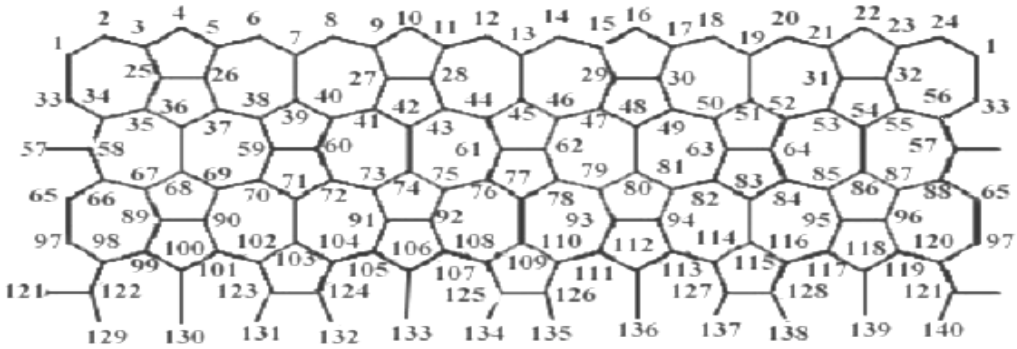


Figure 7. $VC_5C_7[4, 2]$ Nanotube.

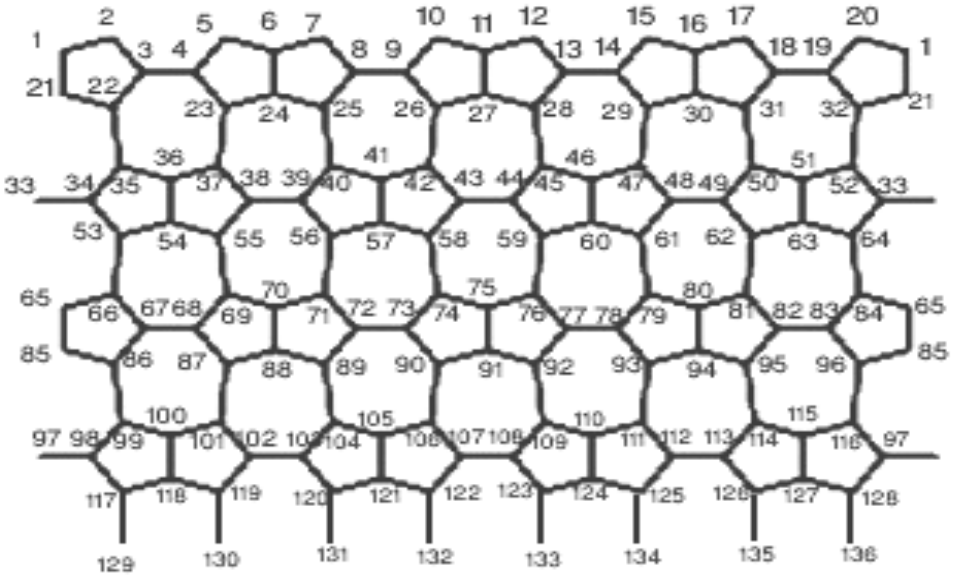


Figure 8. $HC_5C_7[4, 2]$ Nanotube.

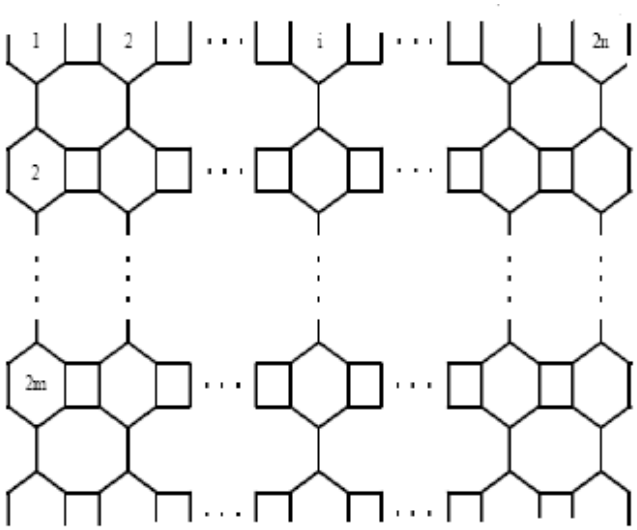


Figure 9. A H-Phenylenic Nanotube.

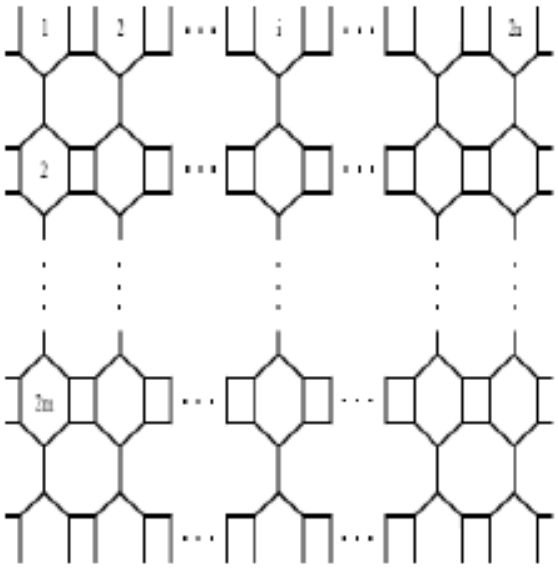


Figure 10. A H-Phenylenic Nanotorus

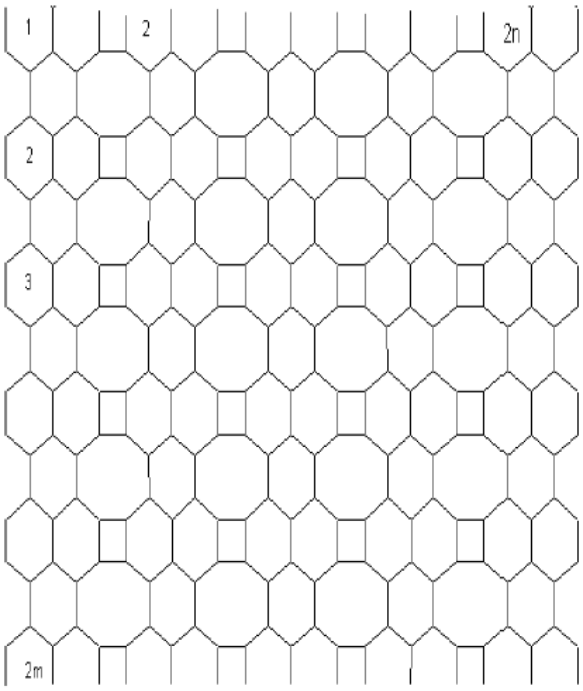


Figure 11. A H- Naphtalenic Nanotube

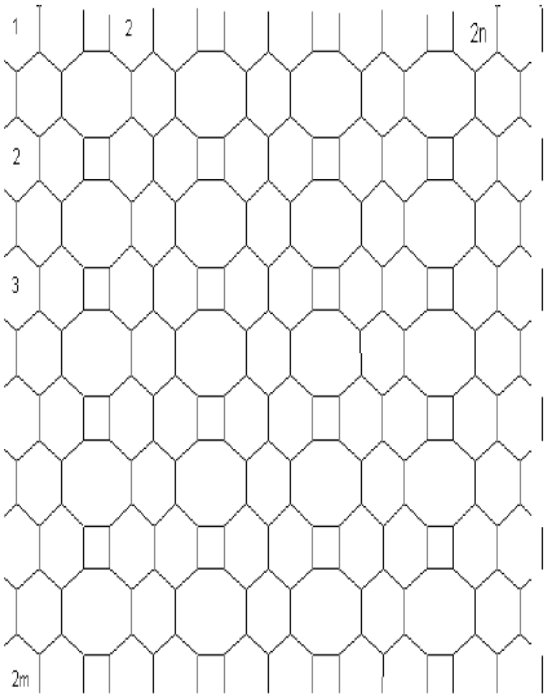


Figure 12. A H- Naphtalenic Nanotorus

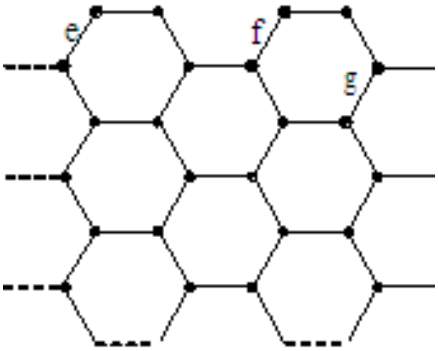


Figure 13. The 2-Dimensional Lattice of a Polyhex Nanotorus.

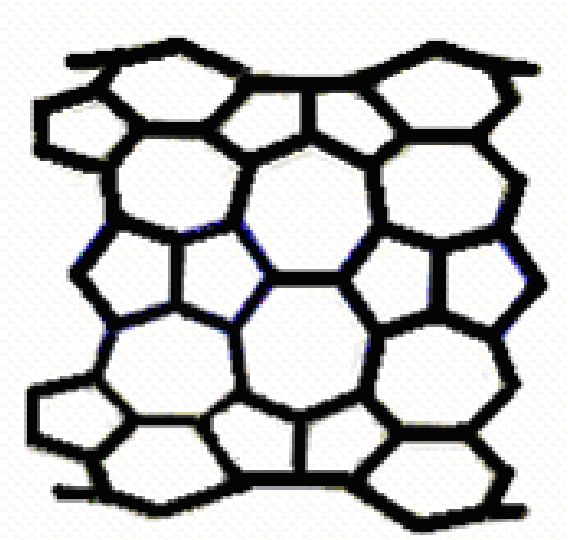


Figure 14. A H C_5C_7 Nanotube.

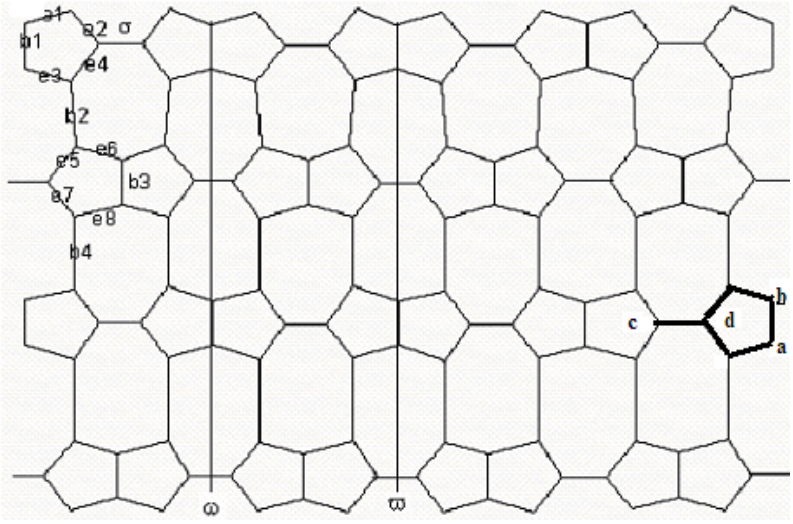
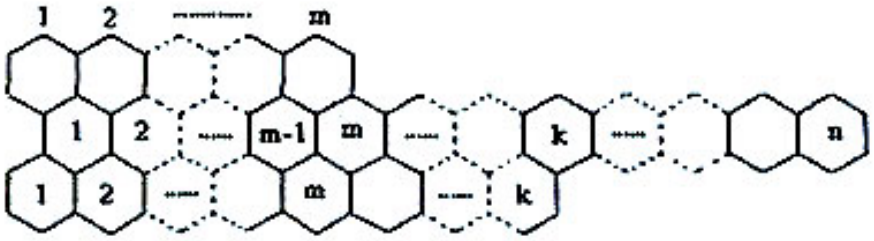
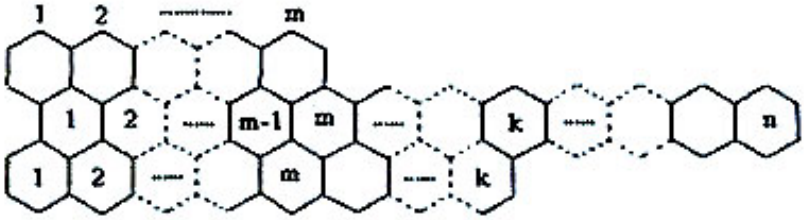


Figure 15. The 2-Dimensional Lattice of HC_5C_7[16,8] Nanotube.

In addition, PI indices of the following systems are also reported in the literature.

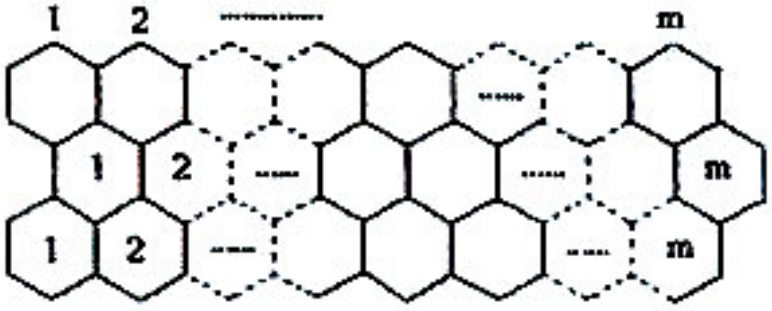


(a) m≤n<k



(b) m<n,k and n ≥k

(c) n≤m and n ≤k



(d) n=m =k

Figure 16. The Pericondenced Benzenoid Graphs Crossing Three Rows of n, m and k in Hexagons.

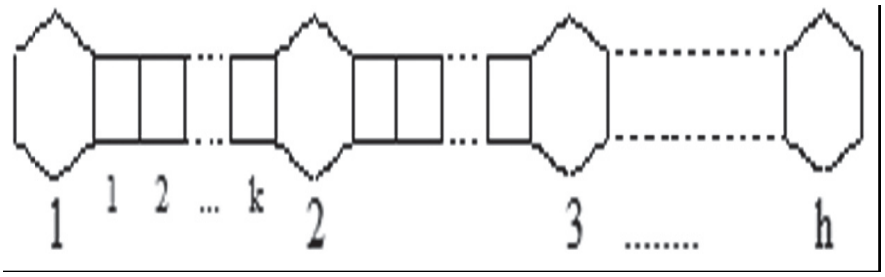


Figure 17. The Graph of Linear Phenylenes.

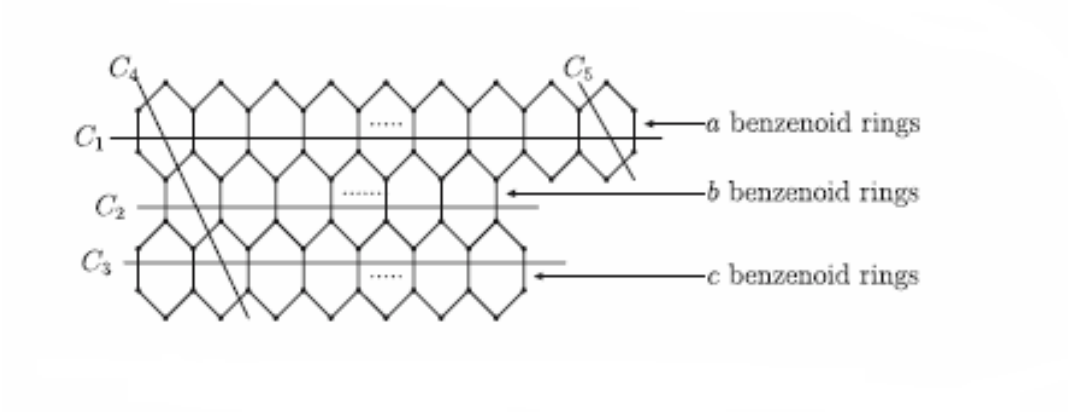


Figure 18. The Graph G(a,b,c) with $b < c \leq a$.

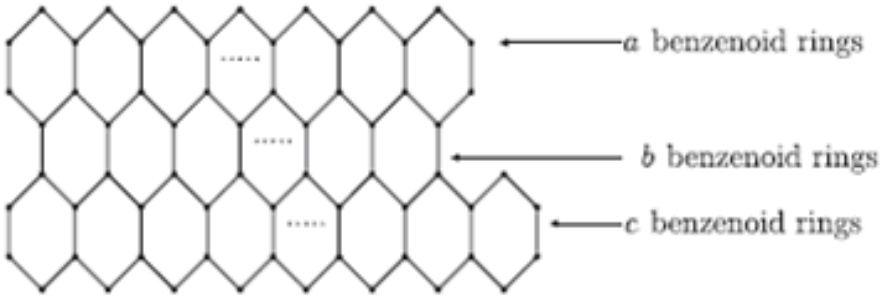


Figure 19. The Graph G(a,b,c).

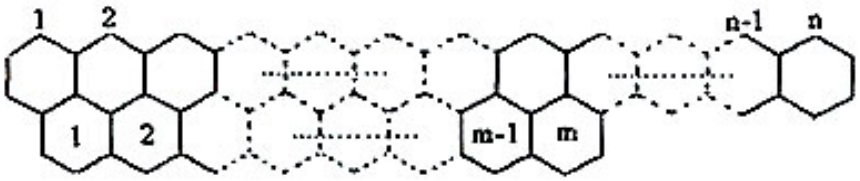


Figure 20. A Pericodenced Benzenoid Graphs Consisting of Two Rows of n and m Hexagons, Respectively, m ≤ n.

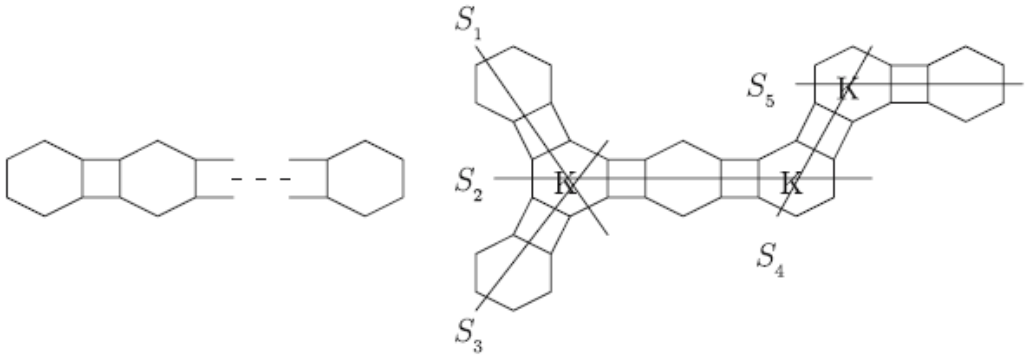


Figure 21. A Linear Chain Phenylene, Kinks, and Segments of a Phenylene.

Figure 22. The Linear Chain Phenylene PH.

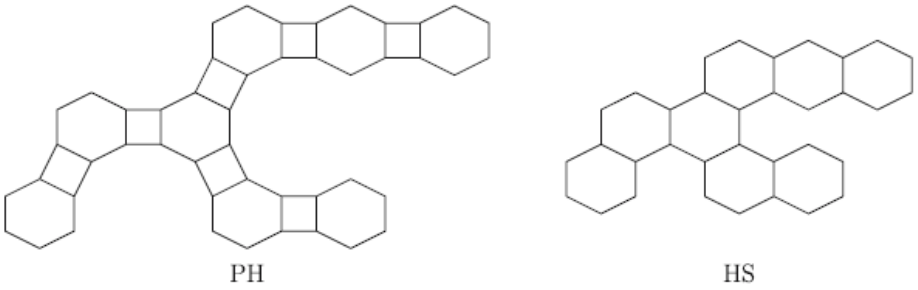


Figure 23. A Phenylene (PH) and Its Hexagonal Square (HS).

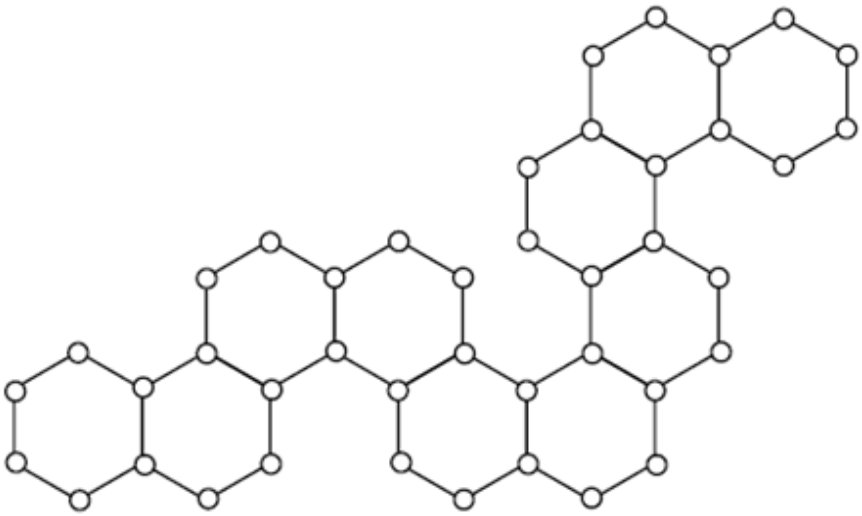


Figure 24. A Fibonacene with h = 10.

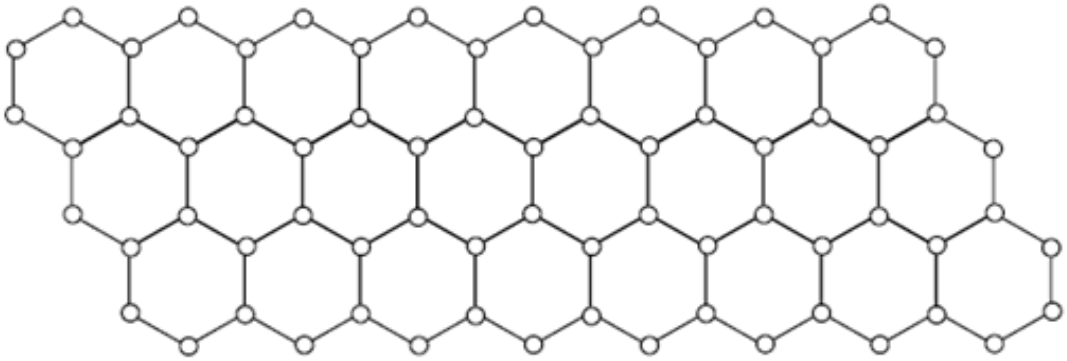


Figure 25. The Parallalogram P(8,3).

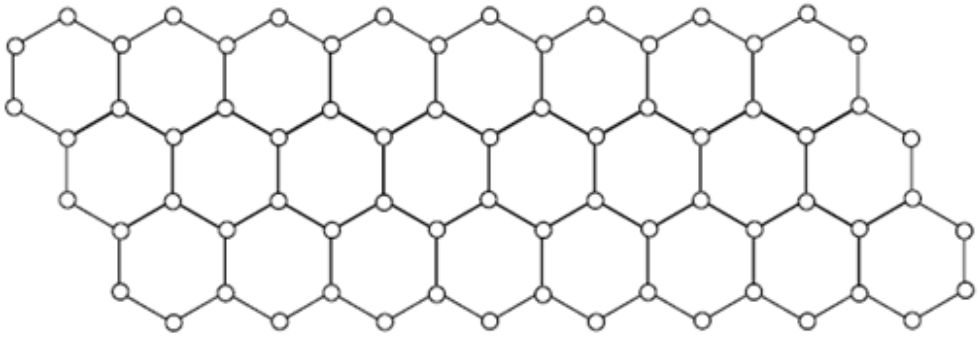


Figure 26. Linear Polycene Parallalogram

4. CONCLUSIONS

The present report indicates that compared to several other topological indices available in the literature, PI index appears to be the best suited topological index for solving problems related to nanotechnology in particular the problems related to carbon nanotubes.

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Table 1. Padmakar-Ivan Index of Nanostructures.

SN	Title	Ref
1	PI Index of zigzag polyhex nanotubes	57
2	PI Index of TU $_4$ C $_8$ (S) polyhex nanotubes	51
3	PI Index of armchair polyhex nanotubes	52
4	Automorphism group and topological indices of the chemical graphs of fullerenes	53,69
5	Computing the PI index of some chemical graphs related to nanostructures	55
6	The PI index of some nanotubes	56
7	PI index of TUV C_6 [2p,q]	84
8	Omega polynomial of tubular nanostructures	86
9	Computing the Szeged and PI indices of VC_5C_7 [p,q] and HC_5C_7[p,q] nanotubes	88
10	PI and Szeged indices of VC_5C_7 [4p,8] nanotubes	59
11	PI Index of polyhex nanotubes	58
12	Computing the Szeged and PI indices of VC_5C_7 [p,w] and HC_5C_7[p,q] nanotubes	88
13	PI polynomial of v-phenylenic nanotubes and nanotori	114
14	PI, Szeged and Edge Szeged indices of infinite family of nanostar dendromers	73
15	Omega and Sadhana polynomial of H-naphthalinic nanotubes and nanotori	87
16	On distance based topological indices of VC_5C_7 [4p,8] nanotubes	59
17	Topological indices of nanotubes,nanotori and nanostars	114
18	Padmakar-Ivan index of H-phenylenic nanotubes and nanotori	115
19	Sadhana : A new topological index for carbon nanotubes (CNTs)	112,113
20	Computing PI index of HAC_5C_6 C_7 nanotubes and nanotori	64
21	Some topological indices of HAC_5 C_7 nanotubes	89
22	PI indices of nanotubes SC_4C_8 [q,2p] covering by C_4 and C_8	55
23	PI index of Some polyhex nanotubes	48,61
24	Computing PI index of zigzag polyhex nanotubes	57,62
25	PI index of v-phenylenic nanotubes and nanotori	63
26	PI and Szeged indices of one pentagonal carbon nanotubes	60
27	Padmakar-Ivan (PI) index of HAC_5 C_7 [r,p]	89
28	Padmakar –Ivan (PI) index of HAC_5 C_7 nanotubes	89
29	PI and Szeged indices of some benzenoid graphs related to nanostructure	50,79
30	PI Index of TUC $_4$ C $_8$ (R) nanotubes	71,90
31	PI Index of C $_4$ C $_8$ (R) nanotubes	74
32	Padmakar-Ivan Index of q-Multi- walled Carbon Nanotubes and Nanotori	65
33	PI Indices of Tori Tp, q [C_4;C_8] Covering C_4 and C_8	82
34	PI Index of Some Nanotubes	49
35	Padmakar-Ivan Index of HAC5C6C7 Nanotubes and Nanotori	78

Table 2. Padmakar –Ivan Index (PI) of Cyclic Graphs Related to Carbon Nanotubes.

SN	Title	Ref
1	PI Index of some benzenoid graphs	50,64,85,91
2	External Catacondensed hexagonal system with respect to the PI index	29
3	The PI index of phenyls	47,75,83
4	On the PI Index: PI partition and Cartesian product graph	76
5	PI Index of product graphs	65,66,72,81
6	Computing PI and Szeged indices of multiple phenylenes and cyclic hexagonal square chain consisting of mutually isomorphic hexagonal chains	67
7	PI indices of pericondensed benzenoid graphs	41
8	A good algorithm for PI index of benzenoid hydrocarbon	91
9	Vertex and edge PI indices of Cartesian product graph	66
10	The vertex PI index and Szeged index of bridge graph	80
11	The PI index of polyamino chains	116
12	The PI index of product graph	65,66,72,81
13	Vertex and edge PI indices of Cartesian products graph	76
14	A matrix method for computing Szeged and vertex PI indices of join and composition of graphs	77
15	The PI index of gated amalgam	116
16	PI polynomial of some benzenoid graphs	54
17	On the PI polynomial of a graph	68
18	Vertex and edge PI indices of product graphs	66
19	On the PI index of Phenylenes and their hexagonal squeezes	75
20	The PI index of bridge and chain graphs	43
21	PI indices of Polyacenes and its use in QSPR	31
22	Relationship and relative correlation potential of the Wiener,Szeged and PI indices	25
23	Novel PI indices of hexagonal chains	30
24	On the estimation of PI index of Polyacenes	47
25	A method of computing the PI index of benzenoid hydrocarbons using orthogonal cuts	33
26	Matrix Method for Computing Szeged and Vertex PI Indices of Join and Composition of Graphs,	77
27	Relationship Between PI and Szeged Indices of a Trinanguline and its Associated Dendrimer	70
28	Some Bounds for PI Indices	92

Table 3. Padmakar – Ivan Index (PI) in Developing QSAR/QSPR/QSTR.

SN	Title	Ref
1	QSAR prediction of toxicity of nitrobenzene	30
2	A novel PI index and its applications to QSPR/QSAR studies	30
3	Use of the PI index in predicting toxicity of nitrobenzene derivatives	93
4	Prediction of ^{13}C Nuclear Magnetic Resonance Chemical Shift ($\sum {}^{13}C_n$) in alkanes and cycloalkanes	94
5	Prediction of lipophilicity of Polyacenes using quantitative structure activity relationship	37
6	A novel method of estimating motor octane number (MON) – A structure property approach	95
7	Novel estimation of lypophilic behavior of polychlorinated biphenyls	96
8	QSAR study of toxicity to aquous organism using the PI index	102
9	QSAR study on solubility of alkanes in water and their partition coefficient in different solvent systems using PI index	97
10	QSAR study on Bioconcentration factor (BCF)of polyhalogenated byphenyls using the PI index	98
11	Correlation between the benzene character of acenes or helicenes and simple molecular descriptors	100
12	QSAR study on ^{13}C NMR Chemical shifts of carbinol carbon atoms	99
13	QSAR study on tadpole narcoses using the PI index: A case of heterogeneous set of compounds	100
14	QSAR study on CA inhibitory activity of disulphonamides : Effect of halogen Substitution	101
15	Carbonic Anhydrase inhibitors: The first QSAR study of inhibition of tumour associated isoenzyme IX with aromatic and heterocyclic systems	103
16	Novel applications of PI index in estimating organic reactivity ;CH –acidity ,S-character and steric Energy	104
17	Novel Applications of PI index : Prediction of the ultrasonic sound velocity in n-alkanes	105
18	Topological estimation of electronic absorption bands of arene absorption spectra as a tool for modeling their toxicity and environmental pollution	64
19	Topological modeling of lipophilicity, diuretic activity and carbonic inhibitory activity of benzene sulphonamides : A molecular connectivity approach	106
20	Novel use of chemical shift in NMR as molecular descriptor: A first report on modeling carbonic anhydrase activity and related parameters	107
21	QSAR studies on benzene sulphonamides carbonic anhydrase inhibition : Need of hydrophobic parameter for topological modeling of binding constants of sulphonamides to Human CA-II	108
22	Use of distance-based topological indices for the estimation of 13 C NMR shifts: A case of benzene derivatives	109
23	Lipophilicity related to carcinogenic activity of aromatic hydrocarbons and heterocyclic verses topological indices	110
24	Topological estimation of aromatic stabilities of Polyacenes and helicenes : Modeling of resonance energy and benzene character	70
25	QSPR correlation of half- wave reduction potentials of cata-condensed benzenoid hydrocarbons	111
26	QSAR studies on inhibitory properties of benzene sulphonamides towards CA I : Dominating role of vander Waals repulsion energy	42
27	PI Indices of polyacenes and their use in QSPR	31
28	Relationship and relative correlation potential of Wiener,Szeged and PI Indices	25

Table 4. Names of institutes working on the applications of PI Index in nanotechnology.

S N	Name of Institute
1	Department of Mathematics ,Univ of Kashan,Tehran
2	Academic centre for education ,Culture and research, Tehran Branch, Tehran,Iran
3	School of Mathematics , Statistics and computer science Tehran Branch, Tehran,Iran
4	Institute of nanoscience and nanotechnology,Univ of Kashan,Tehran
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6	Department of nano materials, Iran color Research Centre (CICRC) Tehran,Iran
7	Faculty of chemistry and chemical engineering, Babes-Bolyai Univ,Cluj,Rommania
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21	A. Irahmanesh: Iran
22	Y. Alizadeh: Iran
23	Hamid Saati: Iran
24	V. Alamiax: Iran
25	B. Edalatzadeh: Iran
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27	Jianxiu Hao: P.R.China
28	O. Khormali: Iran
29	N. Gholami: Iran
30	Sufia Aziz : India
31	Anju Das Manikpuri : India
32	Padmakar V. Khadikar,India
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Table 7. Journals in which papers related to PI index in nanotubes are published.

S N	Name of the Journal
1	Communication in Mathematics and Computer Science (MATCH)
2	J. Chilean Chemical Society
3	Journal of Computational and Theoretical Nanoscience
4	Ars Combinatoria
5	Journal of Physics, Conference Serries
6	Utilitas Mathematica
7	Croatica Chemica Acta
8	The Internet Journal of Nanotechnology
9	Applied Mathematics Letters
10	Journal of Mathematical Chemistry
11	Nanoscience
12	International Journal of Molecular Sciences
13	Journal of Computational Chemistry
14	Digest Journal of Nanomaterial and Biostructures
15	Indian Journal of Chemistry Section A
16	American Journal of Applied Sciences
17	Linear Algebra and its Applications
18	Discrete Applied Mathematics
19	European Journal of Combinatorics
20	Journal of Serbian Chemical Society
21	International Journal of Nanosciences

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